Materials Science

EXAFS ANALYSIS OF FERROELECTRIC SUPERLATTICES, R. Cohen[1], C. Segre*[2], S. Chattopadhyay[2], T. Shibabta[2], Illinois State University[1], Department of Physics, Normal, IL 61790, Argonne National Laboratory[2], Advanced Photon Source, Materials Research and Collaborative Access Team, Argonne, IL 60439, rlcohen@ilstu.edu

Extended x-ray absorption fine structure (EXAFS) is a method used in materials science to explore the local atomic environment in a lattice. Incident x-ray energy is tuned to the binding energy of core-level electrons of the element of choice in the material. Plotting absorption probability as a function of energy shows a sharp absorption peak. As photoelectrons are ejected from the absorbing atom, they are backscattered from other local atoms. Interference from the scattering results in a modulating behavior qualitatively seen as oscillations just beyond the absorption edge. EXAFS compares these oscillations with known atomic models to discern the identities of the backscattering atoms. This study provides a picture of the local atomic environment around Ba atoms in several superlattices containing layers of $SrTiO_3$, $BaTiO_3$, and $CaTiO_3$. A member of the perovskite family, $BaTiO_3$ is a ferroelectric material used in a variety of industrial applications for its piezoelectric properties. The crystallographic structures of $SrTiO_3$ and $CaTiO_3$ are very similar to that of $BaTiO_3$. The motivation for this study is to discover if $BaTiO_3$ will view the other two structures, above and below it respectively, as more $BaTiO_3$. The superlattices could then exhibit uniform ferroelectric properties characteristic of $BaTiO_3$. Preliminary fits of the first three coordination shells show systematic trends in lattice expansion and bond length gradient from the absorbing Ba to the backscattering O and Ti atoms. This may be due to the confined nature of the multilayers, because a superlattice with 8 unit cells of $BaTiO_3$ showed greater lattice expansion than a superlattice with only 4 unit cells.

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